QSAR model for P-gp inhibitor (v1.0)

ProtoADME

ProtoADME is a computational (*in silico*) tool focused on the prediction of endpoints related with the ADME (Absorption, Distribution, Metabolism and Excretion) of chemical substances.

Endpoint

Toxicokinetic: P-gp inhibitor

P-glycoprotein (P-gp, also known as MDR1 or ABCB1) is a member of the superfamily of ABC transporters, which transport various molecules across cellular membranes, and is highly expressed in the intestinal epithelium. P-gp is an energy-dependent efflux pump driven by ATP hydrolysis. Efflux by P-gp can be a major limitation for the oral delivery of a number of drugs.

Metrics

Training set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	378	37
Inhibitor	35	459

Validation set

Experimental values	QSAR predictions	
	Non-inhibitor	**Inhibitor**
Non-inhibitor	135	16
Inhibitor	20	136

Parameters	Training	Validation
Accuracy	0.92	0.88
Sensitivity / recall	0.93	0.87
Specificity	0.91	0.89
Precision	0.93	0.89
Negative predictive value	0.92	0.87
F-score	0.93	0.88
Matthews Correlation Coefficient	0.84	0.77
Critical Success Index	0.86	0.79
Area under the ROC	0.92	0.88